

approaches I will also outline the progress we have made with regard to computational methods in multicomponent crystal prediction as well as property prediction/rationalization.

Keywords: multicomponent crystals, cocrystals, crystal structure prediction

## MS.66.4

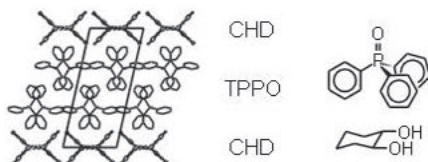
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### An unexpected molecular co-crystal with a variable degree of order

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A 1:1 co-crystal of rac-trans-1,2-C<sub>6</sub>H<sub>10</sub>(OH)<sub>2</sub> (hereafter, CHD) and triphenylphosphine oxide (or, TPPO) has been found that is unusual because there are no strong interactions between the two components. Neither CHD nor TPPO has any obvious packing problem that would make formation of an inclusion complex likely. The TPPO layers are very much like those in two of the four known polymorphs of pure TPPO. The H-bonded ribbons of CHD are similar to those found in other vic-diol crystals. The co-crystals are triclinic (*P1*-bar), with the very small deviations from monoclinic symmetry (*C2/c*) arising from incomplete enantiomeric disorder of the R,R and S,S diols. The sizes of the deviations depend on the solvent from which the crystal is grown. Individual CHD layers seem to be at least mostly ordered. Information about R,R/S,S ordering is transmitted from one diol layer to the next through the almost centrosymmetric TPPO layer. The degree of order is unlikely to change with crystal heating or cooling. Thermal data suggest the existence of the co-crystal is a consequence of kinetic factors. Reasons for this surprising failure of fractional crystallization will be discussed.



Keywords: co-crystal, incomplete ordering, crystal growth

## MS.66.5

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### In-situ cocrystallisation combined with Raman spectroscopy

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Fast characterization of the products from cocrystallisation experiments is highly important since there are no general rules for appropriate growth conditions. Therefore a large number of experiments have to be performed to find the right conditions which favor the growth of a cocrystal over the growth of the individual components. For in-situ crystallization on a single crystal diffractometer this is especially important as characterization by diffraction is time consuming. We therefore incorporated a Raman probe into our in-situ laser zone melting apparatus. First results from systems containing acetylene, dioxane, formamide, formic acid and formaldehyde are highly promising. Already in the Raman spectra of the liquid mixtures we found hints to the formation of

molecular aggregates which might be precursors of the cocrystals. After solidification and zone melting growth we used Raman spectroscopy to identify the formation of a cocrystal. Basic research in cocrystal formation is of increasing interest to pharmaceutical science as cocrystals of active pharmaceutical ingredients can have advantageous properties.

Keywords: crystal growth, ocrystallization and complexation of small molecule, raman spectroscopy

## MS.67.1

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### Magnetic and structural transitions in frustrated magnets

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I will review recent neutron and synchrotron X-ray scattering studies of frustrated spinels and kagomes. The main focus will be to investigate what kinds of magnetic transitions, and lattice and magnetic states can arise when frustrated spins are coupled with lattice in the highly frustrated antiferromagnets.

Keywords: frustrated magnets, neutron scattering, X-ray scattering

## MS.67.2

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### E/T-scaling behavior in the magnetic quasicrystal Zn-Mg-Ho

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Quasicrystals have distinct (quasiperiodic) spatial symmetry characterized by a hidden translational invariance in higher dimensional space, and thus differs both from the periodic crystals and random glasses. Ordering and dynamics of spins in the quasiperiodic structures have been one of fundamental issues. Despite a variety of theoretically expected anomalous properties, earlier macroscopic experiments only exhibited rather normal spin-glass-like behavior. Recently, using the neutron scattering technique, we have revealed non-trivial spin dynamics --temperature independent spin excitation spectrum-- in the magnetic quasicrystal Zn-Mg-Ho, which is, we believe, the most prominent feature ever found. Magnetic excitation spectrum in the Zn-Mg-Ho quasicrystal has only a quasielastic component centered at the elastic position. The quasielastic signal for the positive energy-transfer side is found to be temperature-independent in a wide temperature range  $1.5 < T < 200\text{K}$ ; it may be noteworthy that the excitation spectrum shows little change even below the spin-glass-like freezing temperature  $T = 1.95\text{K}$ . In the low-energy region  $E < 1.5\text{meV}$ , imaginary part of generalized susceptibility obtained from the scattering function shows scaling behavior:  $\text{Im } \chi(Q, E/k_B T)(k_B T)^{1/3} \propto (E/k_B T)^{-1/3} \tanh(\alpha E/k_B T)$ . This is a typical *E/T*-scaling function, where the susceptibility is scaled only by *E/T*, except for the weak prefactor  $T^{1/3}$ . This *E/T*-scaling is frequently observed in the non-Fermi-liquid (NFL) compounds, such as UCu<sub>4</sub>Pd, being in vicinity of